#### Benzoic acid, 3,6-dichloro-2-hydroxy-3401-80-7 | DTXSID9041657

3401-80-7	DIXSID9041657	

# **Model Performance**

Model	Data

# Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

# Model Results

Predicted value: 224 °C

Global applicability domain: Inside

Local applicability domain index: 6.38e-01

Confidence level: 6.13e-01

# Nearest Neighbors from the Training Set

#### Image not found

3,5-Dichlorosalicylic acid

Measured: 221 Predicted: 223

# Image not found

Benzoic acid, 3,5-dibromo-2-

hydroxy-

Measured: 228 Predicted: 228

#### Image not found

Benzoic acid, 3,5-dichloro-4-

hydroxy-

Measured: 265 Predicted: 247

#### Image not found

Benzoic acid, 2-hydroxy-3,5-

diiodo-

Measured: 236 Predicted: 230

#### Image not found

Benzoic acid, 5-chloro-2-

hydroxy-

Measured: 172 Predicted: 186